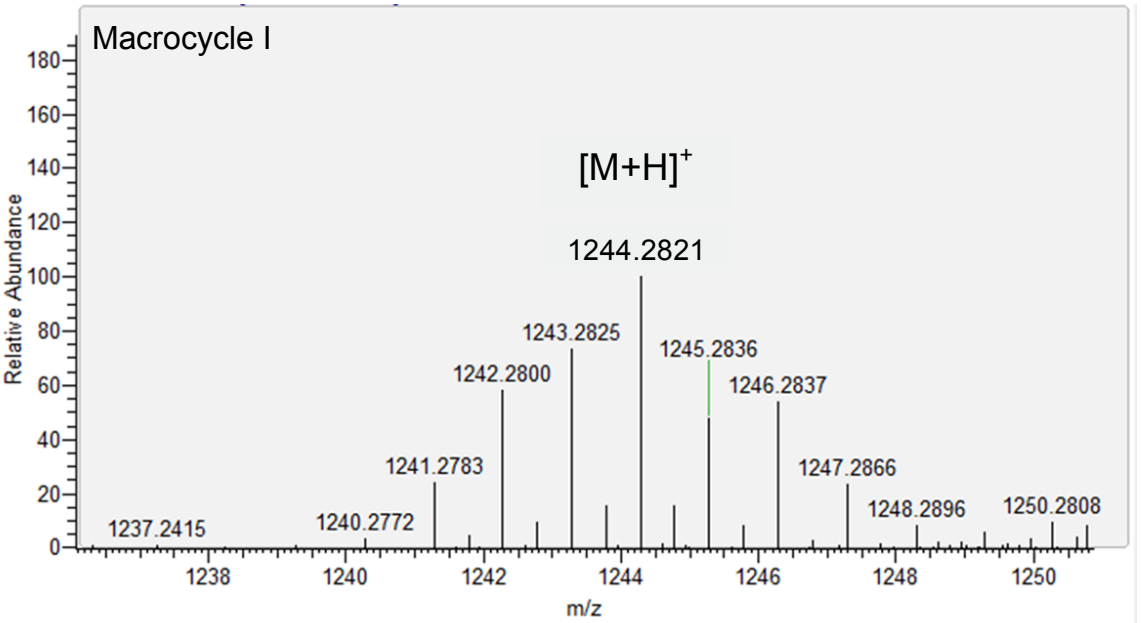
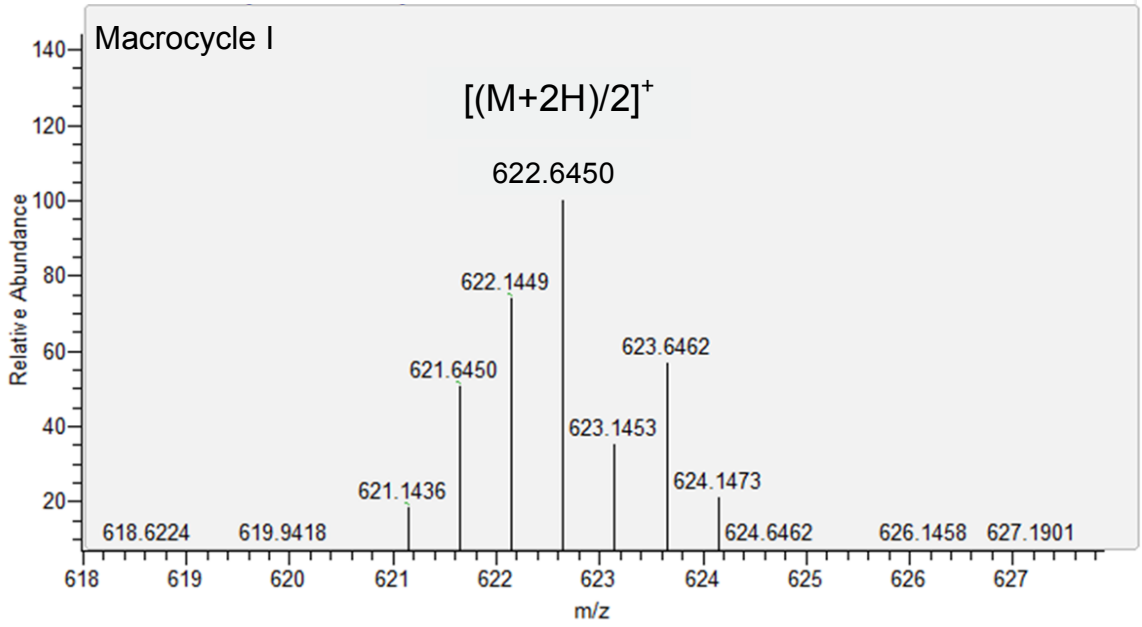
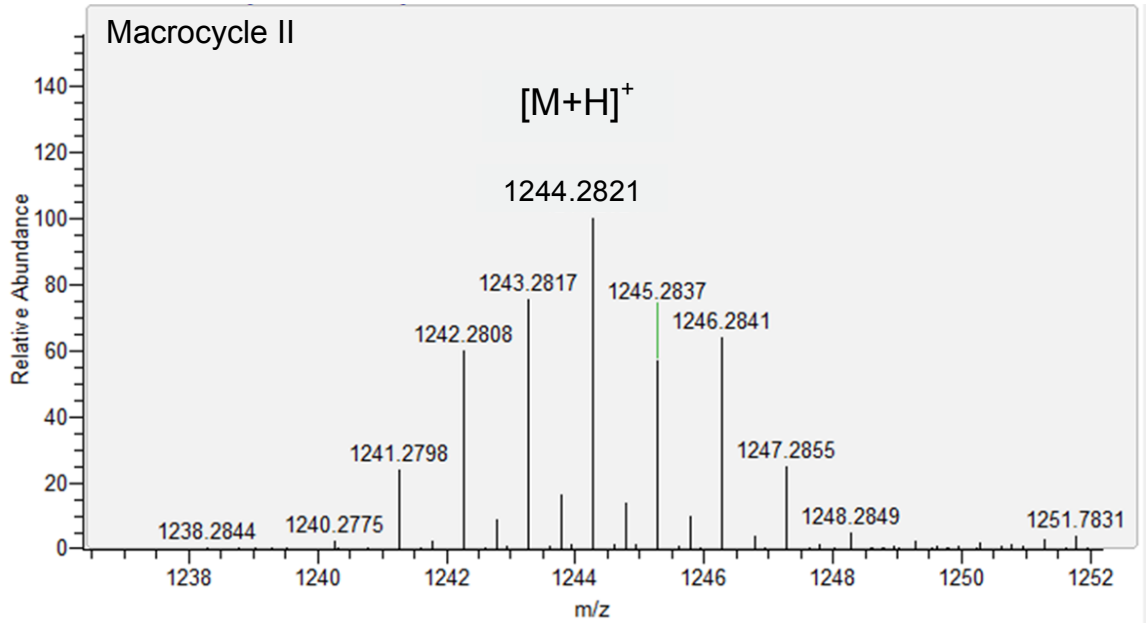
Supporting Information

A)





B)


Macrocycle II
[M+H]+
1244.2821
1243.2817
1245.2837
1246.2841
1242.2808
1241.2798
1247.2855
1238.2844
1240.2775
1248.2849
1251.7831
Relative Abundance
m/z

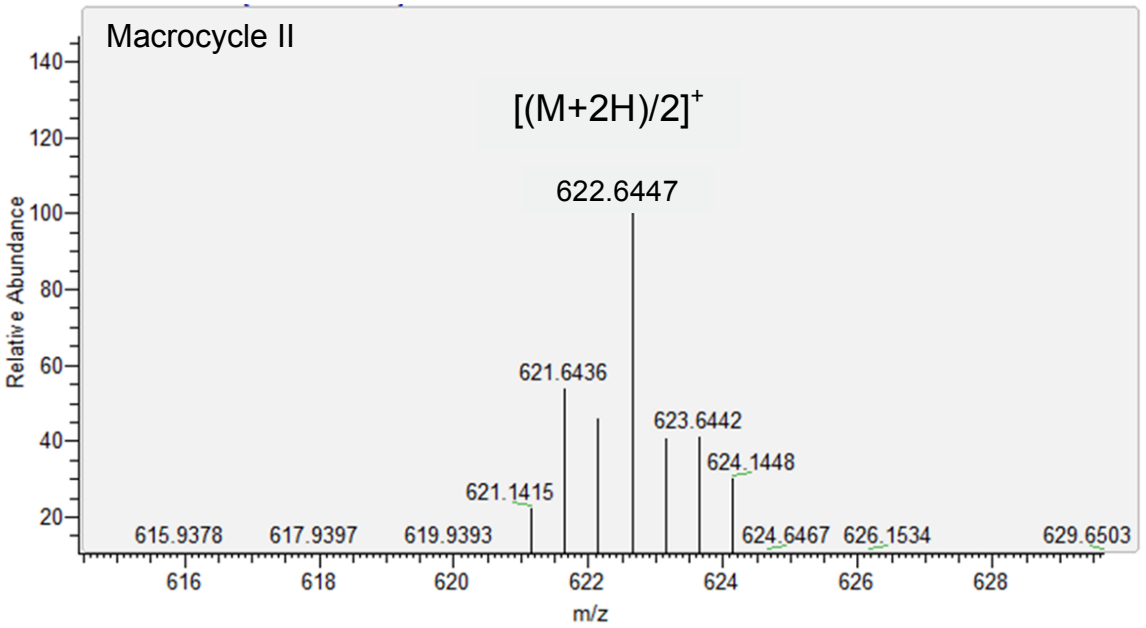

Macrocycle II
[(M+2H)/2]+
622.6447
621.6436
623.6442
624.1448
621.1415
615.9378
617.9397
619.9393
624.6467
626.1534
629.6503
Relative Abundance
m/z

Figure S1.

HRMS of cyclized products of macrocycle I and II. A) HRMS of macrocycle I: calculated for C49H58GdN12O11S3 [(M+H)+]: 1244.2751, observed. HR-ESI/MS: m/z 1244.2821; calculated for C49H59GdN12O11S3 [(M+2H)/2]+: 622.6415, observed. HR-ESI/MS: m/z 622.6450. B) HRMS of macrocycle II: calculated for C49H58GdN12O11S3 [(M+H)+]: 1244.2751, observed. HR-ESI/MS: m/z 1244.2821; calculated for C49H59GdN12O11S3 [(M+2H)/2]+: 622.6415, observed. HR-ESI/MS: m/z 622.6447.

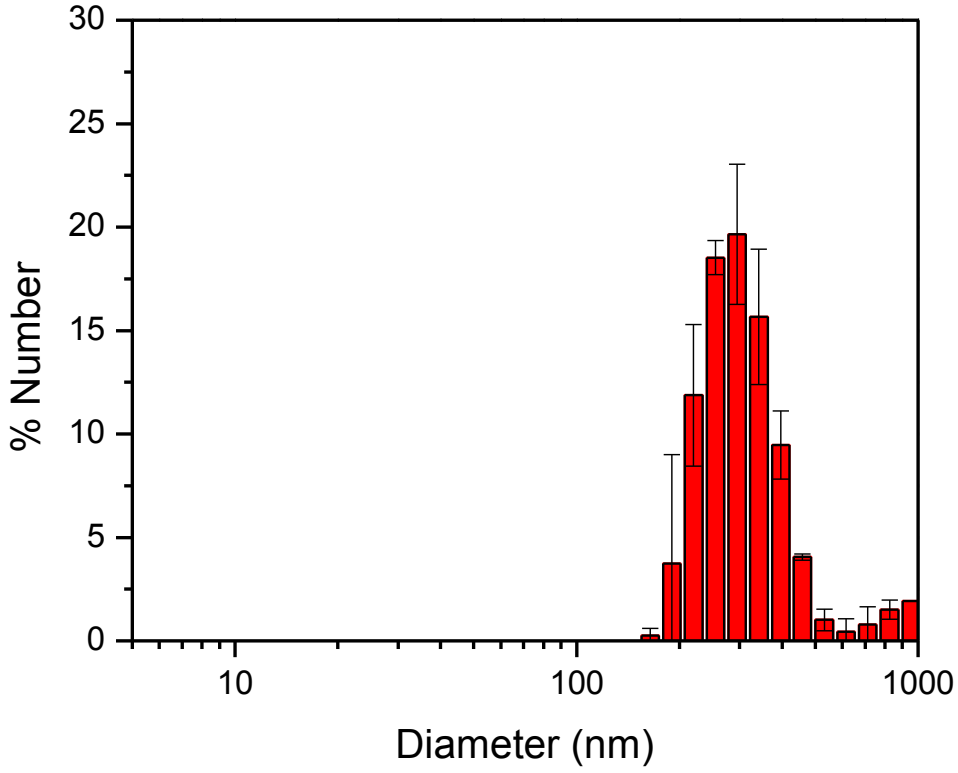


Figure S2.

DLS analysis of C-SNAM (200 μM) following incubation with caspase-3 (50 nM) in caspase buffer (pH 7.4) overnight. Error bars indicated standard deviation, coming from two repeated measurements.

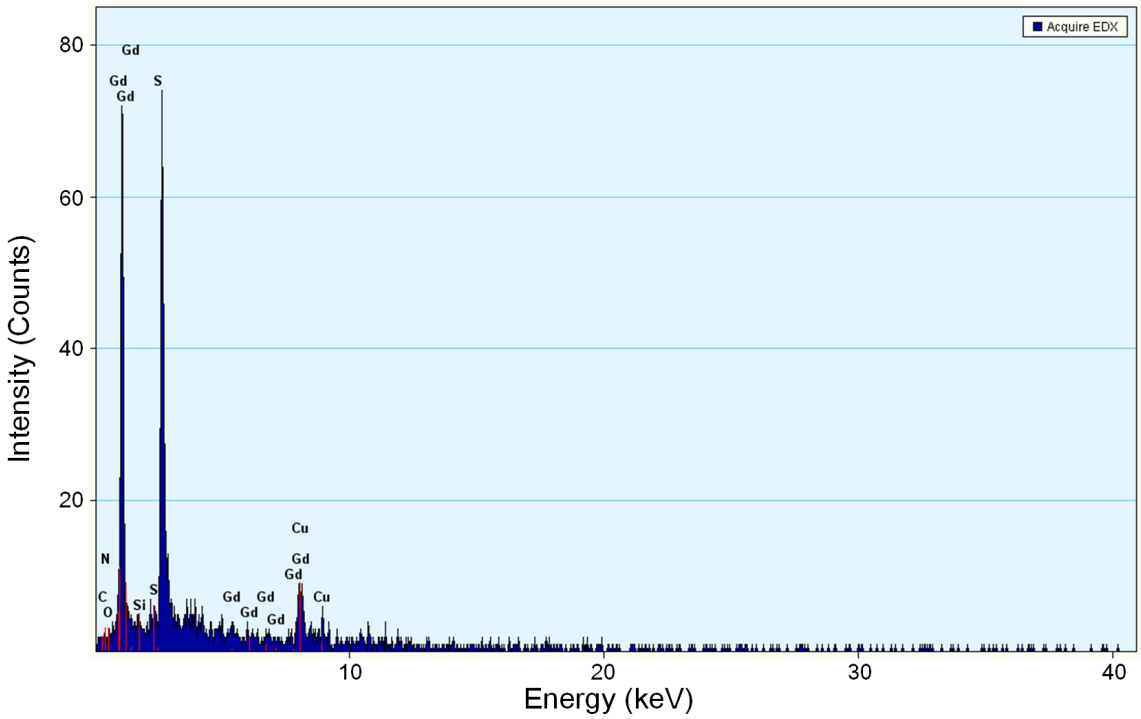


Figure S3.

Energy-dispersive X-ray (EDX) spectroscopy analysis of the nanoparticles in Fig. 1c shows the presence of Gd element signal from the particles.

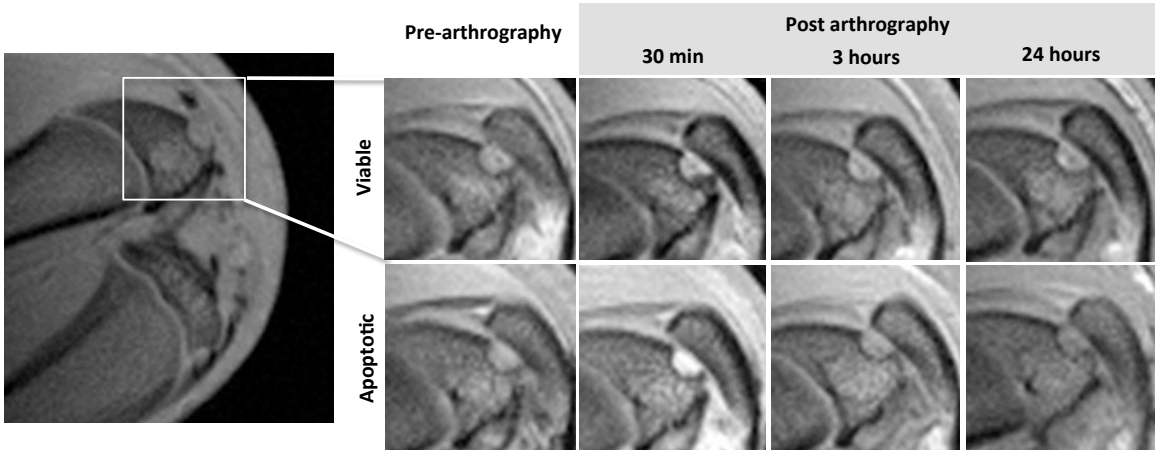


Figure S4

*In vi*vo MRI of viable and apoptotic rASC implants. T1 weighted MR imaging of the viable and apoptotic rASCs before, 30min, 3 hours, and 24 hours after intra-articular injection of the C-SNAM.